Spin dependent attenuation lengths in ferromagnets

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Spin dependent attenuation lengths (AL) as a function of the hot electron energy are calculated for Fe, Co, and Ni. If $\lambda^{-1}(\lambda^{-1})$ is the AL of an electron with spin parallel (antiparallel) to the majority spin direction of the ferromagnet then the quantity $A = (\lambda^{-1} - \lambda^{-1})/(\lambda^{-1} + \lambda^{-1})$ is found to change sign as a function of the electron energy.

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The attenuation lengths (AL) of hot electrons in a ferromagnetic material may be spin dependent because the majority spin electron density differs from the minority density and only electrons of parallel spin undergo an exchange interaction. It has been pointed out by DeWames and Vredevoe(1) and more recently by Bringer et al(2) that the spin dependence of the electron AL may be an important factor in the interpretation of photoemission experiments which measure the spin polarization of the photoexcited electrons. We find that the work of Bringer et al(2) and Feder(3) greatly overestimates the AL asymmetry, given by $A=(\lambda^2-\lambda^2)/(\lambda^2+\lambda^2)$, and in fact it usually gives the wrong sign for this quantity. Our conclusion is that the spin dependence of the AL cannot explain the anomalously high values of the spin polarization of the photoyield measured by Bringer et al(2) and in fact similar experiments on Co do not produce an anomalous result(4).

In addition, the elastic scattering of polarized electrons from a Ni surface has been measured in a very elegant experiment by Celotta et al(5) who observed an asymmetry in the scattered electrons. The most appealing interpretation of their results is that the asymmetry results from the exchange interaction between the scattered electrons and those of Ni. However, it could also result from the spin dependence of the electron AL. From the small magnitude we calculate for A in Ni it can be concluded that the results of the polarized electron scattering from Ni obtained by Celotta et al(5) cannot be explained by a spin dependent AL.

Our calculations of the spin dependent AL for Fe, Co and Ni are based on the statistical approximation introduced by Lindhard et al(6) who calculated the energy loss of charged particles in a variety of materials. It has recently been employed by Tung et al(7) to calculate the electron AL for Al, Si, Ni, Cu, Ag and Au with very good results. The statistical approximation bears some resemblance to the local density approximation; the electrons in a volume element of the metal are characterized by a local density and the contribution of those electrons to the scattering of a hot electron (i.e., to $\lambda^{-1}(\mathbf{r})$) is taken to be that of a free electron gas of the same density, λ_F^{-1} . The total inverse AL (IAL) is obtained by integrating λ_F^{-1} over the Wigner-Seitz cell of the metal.

We choose the interaction between antiparallel spin electrons to be the Coulomb interaction screened by the Lindhard dielectric function and that between parallel spin electrons to be the antisymmetrized screened (Lindhard) Coulomb interaction. This represents an extension of the work of Ritchie and Ashley(8) who calculated the effects of exchange on the AL of low energy electrons in a free electron gas; for energies $\mathbb{E} \cdot 1 \cdot 1 \cdot \mathbb{E}_{\xi}$ dynamic screening can be neglected. We present calculations of the AL for energies up to 200eV above \mathbb{E}_{ξ} for free electron materials with a wide range of densities. The results of these calculations are then applied to magnetic materials by use of the statistical approximation.

Let a hot electron with momentum \overrightarrow{p}_o , energy $\varepsilon_{\overrightarrow{p}_o}$ and spin σ interact with an electron from the solid and scatter into the final state \overrightarrow{p}_f , $\varepsilon_{\overrightarrow{p}_f}$, σ . The electron from the solid scatters from \overrightarrow{l}_o , $\varepsilon_{\emph{k}_f}$, σ' to \overrightarrow{l}_f , $\varepsilon_{\emph{k}_f}$, σ' . The scattering rate for this event in the Born approximation is given by

 $\mathbf{P}^{\sigma}(\mathbf{p}_{o}) = \frac{2\pi}{\hbar} \sum_{\ell_{o}, \ell_{f}, \mathbf{p}_{f}, \sigma} (1 - \mathbf{f}_{\mathbf{p}_{f}\sigma}) (1 - \mathbf{f}_{\ell_{f}\sigma}') \mathbf{f}_{\ell_{o}\sigma}'$

$$\times |U(|\stackrel{\rightarrow}{p}_{o} - \stackrel{\rightarrow}{p}_{f}|, \varepsilon_{p_{o}} - \varepsilon_{p_{f}}) - \delta_{\sigma\sigma}, U(|\stackrel{\rightarrow}{p}_{o} - \stackrel{\downarrow}{k}_{f}|, \varepsilon_{p_{o}} - \varepsilon_{\ell_{f}})|^{2}$$
 (1)

$$\mathbf{x}\delta(\overset{\rightarrow}{\mathbf{p}_{o}}+\overset{\rightarrow}{\mathbb{A}_{o}}-\overset{\rightarrow}{\mathbf{p}_{f}}-\overset{\rightarrow}{\mathbb{A}_{f}})\delta(\varepsilon_{\overset{\rightarrow}{\mathbf{p}_{o}}}+\varepsilon_{\overset{\rightarrow}{\mathbf{A}_{o}}}-\varepsilon_{\overset{\rightarrow}{\mathbf{p}_{f}}}-\varepsilon_{\overset{\rightarrow}{\mathbf{A}_{f}}})$$

where $U(q,\omega)$ is the dynamically screened electron-electron interaction and f is a Fermi function. We use Eq. (1) to study the free electron case by taking $U(q,\omega) = \mathbf{v}_q / \epsilon(q,\omega)$ where the Coulomb potential \mathbf{v}_q is screened by the Lindhard dielectric function(9) $\epsilon(q,\omega)$, which neglects exchange and correlation. Thus the effects of exchange are taken into account through the antisymmetrization in Eq. (1).

The interaction in Eq. (1) is antisymmetric in the electron coordinates in the case where the incident hot electron spin is parallel to the spin of the interacting electron in the solid $(\sigma'=\sigma)$. The contribution to Eq. (1) when the spins are antiparallel $(\sigma'=\overline{\sigma})$ can be written as

$$P_{D}^{\sigma\sigma}(P_{O}) = \frac{a_{O}^{-1}}{2\pi} \frac{\varepsilon_{f}}{\varepsilon_{p}} \int_{0}^{x_{m}} dx_{1} \int \frac{dz_{1}}{z_{1}} \operatorname{Im}(\frac{-1}{\varepsilon(x_{1}, z_{1})})$$
 (2)

where
$$x_1 = (\epsilon_{p_0} - \epsilon_{p_f})/\epsilon_f$$
, $x_m = (\epsilon_{p_0} - \epsilon_f)/\epsilon_f$, $z_1 = |\stackrel{\rightarrow}{p_0} - \stackrel{\rightarrow}{p_f}|/2k_f$

and a is the Bohr radius. Eq. (2) measures the scattering into electron-hole pairs and plasmons without exchange scattering, and was originally derived by Quinn and Ferrell(10). When the spins are parallel the contribution to Eq. (1) from the interference between direct and exchange scattering can be written as

$$P_{I}^{\sigma\sigma}(p_{o})=$$

$$\frac{a_{0}^{-1}}{(2\pi)^{2}} \frac{h}{2ma_{0}} \frac{\epsilon_{f}}{\epsilon_{p_{0}}} \int dx_{1} \int dx_{2} \int \frac{dz_{1}}{z_{1}^{2}} \int \frac{dz_{2}}{z_{1}^{2}} g(x_{1}, z_{1}; x_{2}, z_{2})$$
(3)

 $g(x_1,z_1;x_2,z_2)=$

$$[\operatorname{Im}(\frac{-1}{\epsilon(\mathtt{x}_1,\mathtt{z}_1)})\operatorname{Im}(\frac{-1}{\epsilon(\mathtt{x}_2,\mathtt{z}_2)}) + \operatorname{Re}(\frac{-1}{\epsilon(\mathtt{x}_1,\mathtt{z}_1)})\operatorname{Re}(\frac{-1}{\epsilon(\mathtt{x}_2,\mathtt{z}_2)})]$$

$$x[1-\alpha^{2}(x_{1},z_{1})-\alpha^{2}(x_{2},z_{2})]^{-1/2}$$
(4)

$$\alpha(x,z)=(x+4z^2)[4(p_0/k_f)z]^{-1}$$
 (5)

The exchange scattering process provides the extra momentum and energy transfer, x_2 =(ϵ_p_o - ϵ_f)/ ϵ_f and $z_2 = |\vec{p}_0 - \vec{k}_f|/2k_f$, in this expression. Momentum and

energy conservation impose restrictions on the integrations in Eq. (3).

Parallel spin scattering also contributes a term $P_D^{\sigma\sigma}(p_0)$ identical to Eq. (2) and the total scattering

$$P^{\sigma}(p_{o}) = [P_{D}^{\sigma\sigma}(p_{o}) + P_{D}^{\sigma\overline{\sigma}}(p_{o})] - P_{I}^{\sigma\sigma}(p_{o})$$
(6)

where $P_D^{\sigma\sigma}(p_0) = P_D^{\sigma\sigma}(p_0)$, and the minus sign arises because $P_{\scriptscriptstyle T}$ is due to an interference term.

The free electron metal is unpolarized so that $\lambda^{-1}_{\ \ \uparrow} = \lambda^{-1}_{\ \ \downarrow}$. To relate the free electron results to

ferromagnetic metals, we use the density-functional calculations of Moruzzi et al(11) for the charge densities of majority and minority spins in Fe, Co and Ni. Following the statistical approximation we average λ^{-1} over the Wigner-Seitz cell, at each point using the free electron value of λ^{-1} corresponding to the ferromagnetic density at that point. The quantities of interest are the IAL both with and without the new exchange interference term, and the difference between the IAL for incident electrons with spin parallel (λ^{-1}) and antiparallel (λ^{-1}) to the majority spins. To calculate the IAL's we average over the paramagnetic state of the metal since the spin dependence of the IAL's is a second order effect. calculate the difference in IAL's we expand the free electron IAL about the paramagnetic state before averaging to find

$$\lambda^{-1}_{\uparrow}(\mathbf{n}_{\uparrow}) - \lambda^{-1}_{\downarrow}(\mathbf{n}_{\downarrow})^{\sim}_{\downarrow} \frac{-\partial \lambda_{\underline{\mathbf{I}}}^{-1}}{\partial \mathbf{n}} \Big|_{\mathbf{n}_{\underline{\mathbf{p}}}}(\mathbf{n}_{\uparrow} - \mathbf{n}_{\downarrow})$$
 (7)

where $n_{p}=n_{p}+n_{p}$. Here only the interference term enters the spin-dependent difference. The sign of $\partial \lambda^{-1}/\partial n$ depends on incident electron energy. At very high energies the scattering rate increases with the number of scatterers so that $3\lambda_T^{-1}$ /0n>0 as expected intuitively. At very low energies, momentum transfers are limited to $q \underline{\leq} 2k_{\mbox{\scriptsize f}}$ and the Coulomb potential

 $\mathbf{v}_{\mathbf{q}}$ causes this feature to dominate the scattering rate. Decreasing the density of an electron gas requires a smaller k_f so that the scattering rate increases and $\partial \lambda_I^{-1}/\partial \bar{n} < 0$. This behavior is well known

for the direct term, Eq. (2). Since $(n_{\downarrow}-n_{\downarrow})$ is positive over most of the Wigner-Seitz cell, then the asymmetry, A, is negative at high energies (i.e., $\lambda^{+} > \lambda^{+}$) and positive at low energies (i.e., $\lambda^{+} > \lambda^{+}$). This is shown for Fe, Co and Ni in Fig. (1). For the case of Ni, the presence of the s and p bands cause a predominance of minority spin density close to the outer portion of the Wigner-Seitz cell(11) so that at very low energies A changes sign a second time.

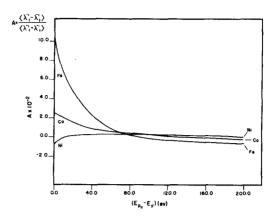


Fig. 1. Calculated difference of IAL for incident electron with spin parallel and antiparallel to majority spins of Fe, Co and Ni as a function of incident electron energy.

REFERENCES

- 1) R. E. DeWames and L. A. Vredevoe, Phys. Rev. Lett. 23, 123 (1969).
- A. Bringer, M. Campagna, R. Feder, W. Gudat, E. Kisker, and E. Kuhlmann, Phys. Rev. Lett. 42, 1705 (1979).
- R. Feder, Solid State Comm. 31, 821 (1979).
- M. Campagna, private communication.
- R. J. Celotta, D. T. Pierce, G. C. Wang, G. D. Bader and G. P. Felcher, Phys. Rev. Lett. 43, 728 (1979).
- J. Lindhard and M. Scharff, Rgl Danske Videnskab. Selakab, Mat.-Fys. Medd. 27, No. 15 (1953). J. Lindhard, M. Scharff and H. E. Schiftt, Kgl. Danske Vindenskab. Selskab., Mat.-Fys. Medd. 33, No. 14 (1963).
- C. J. Tung, J. C. Ashley and R. H. Ritchie, Surface Sci. 81, 409 (1979).
- R. H. Ritchie and J. C. Ashley, J. Phys. Chem. Solids 26, 1689 (1965).
- J. Lindhard, Kgl. Danske Videnskab. Selskab., Mat.-Fys. Medd. <u>28</u>, No. 8 (1954). J. J. Quinn and R. A. Ferrell, Phys. Rev. <u>112</u>,
- 812 (1958).
- V. L. Moruzzi, J. F. Janak, and A. R. Williams, "Calculated Electronic Properties of Metals," Pergamon Press Inc.